Supplementary material

Table S1. Total energies (in au) of the G2 test set (148 molecules) obtained from BLYP, OLYP, B3LYP and O3LYP. G2 geometries and 6-311+G(3df,2p) basis sets are used. All calculations are done with Jaguar 4.0

No.	Molecule	E(BLYP)	E(OLYP)	E(B3LYP)	E(O3LYP)
1	H_2	-1.1695419	-1.1744281	-1.1799916	-1.1782284
2	LiH	-8.0701814	-8.0728302	-8.0862482	-8.0776528
3	BeH	-15.2474116	-15.2515316	-15.2657980	-15.2555773
4	CH	-38.4786588	-38.4774826	-38.4958674	-38.4781674
5	CH_2 ($^3B_1$)	-39.1424547	-39.1489553	-39.1678211	-39.1527466
6	CH_2 ($^1A_1$)	-39.1266833	-39.1278032	-39.1500245	-39.1310141
7	CH_3	-39.8265709	-39.8327297	-39.8577816	-39.8391602
8	CH_4	-40.4992339	-40.5088800	-40.5367731	-40.5176927
9	NH	-55.2266492	-55.2255713	-55.2432159	-55.2243983
10	NH_2	-55.8836050	-55.8823900	-55.9045845	-55.8830361
11	NH_3	-56.5600089	-56.5628791	-56.5868165	-56.5656392
12	OH	-75.7528521	-75.7415629	-75.7655583	-75.7380815
13	H_2O	-76.4464441	-76.4392460	-76.4632002	-76.4369147
14	HF	-100.4757262	-100.4606986	-100.4857287	-100.4548477
15	SiH_2 ($^1A_1$)	-290.6176223	-290.6153567	-290.6434980	-290.6064927
16	SiH_2 ($^3B_1$)	-290.5833251	-290.5888436	-290.6105558	-290.5795637
17	SiH_3	-291.2303516	-291.2336806	-291.2646049	-291.2280712
18	SiH_4	-291.8766042	-291.8787815	-291.9183106	-291.8769877
19	PH_2	-342.5124669	-342.5205049	-342.5390923	-342.5084319
20	PH_3	-343.1454507	-343.1554626	-343.1786113	-343.1461398
21	H_2S	-399.4020428	-399.4202715	-399.4287796	-399.4046088
22	HCl	-460.8166789	-460.8420822	-460.8384843	-460.8210171
23	Li_2	-14.9938798	-15.0037898	-15.0158670	-15.0081740
24	LiF	-107.4575733	-107.4356838	-107.4715718	-107.4306058
25	C_2H_2	-77.3298683	-77.3298253	-77.3610053	-77.3294128
26	$H_2C=CH_2$	-78.5732599	-78.5805718	-78.6209721	-78.5870945
27	H_3C-CH_3	-79.7970034	-79.8122240	-79.8614760	-79.8258302
28	CN	-92.7322723	-92.7250769	-92.7424548	-92.7133464
29	HCN	-93.4384706	-93.4319858	-93.4579720	-93.4248045
30	CO	-113.3432334	-113.3287347	-113.3553269	-113.3174980
31	HCO	-113.8812509	-113.8695449	-113.8981972	-113.8599640
32	$H_2C=O$	-114.5232708	-114.5144454	-114.5486929	-114.5086769
33	CH_3-OH	-115.7300397	-115.7265632	-115.7728756	-115.7288284
34	N_2	-109.5532249	-109.5417741	-109.5626406	-109.5285425
35	H_2N-NH_2	-111.8757876	-111.8756242	-111.9172447	-111.8765265
36	NO	-129.9314945	-129.9153576	-129.9390043	-129.9000195
37	O_2	-150.3770344	-150.3565775	-150.3770660	-150.3361156
38	HO-OH	-151.5958814	-151.5720949	-151.6114767	-151.5599480
39	F_2	-199.5830984	-199.5417633	-199.5806299	-199.5200668
40	CO_2	-188.6453052	-188.6224794	-188.6588704	-188.6017883
41	Na_2	-324.5783835	-324.5620582	-324.6008854	-324.5437723
42	Si_2	-578.8782091	-578.8713707	-578.8995927	-578.8392566
43	P_2	-682.7267955	-682.7318635	-682.7480225	-682.6937597
44	S_2	-796.4092860	-796.4347266	-796.4330312	-796.3907617
45	Cl_2	-920.3961945	-920.4380318	-920.4245700	-920.3899529
46	NaCl	-622.5744314	-622.5844212	-622.6043116	-622.5542595
47	SiO	-364.7714960	-364.7464316	-364.7831614	-364.7226138
48	CS	-436.2384839	-436.2491447	-436.2570594	-436.2226613
49	SO	-473.4141423	-473.4125596	-473.4257512	-473.3808472
50	ClO	-535.3519390	-535.3583100	-535.3646436	-535.3236616
51	ClF	-560.0123220	-560.0117981	-560.0264578	-559.9776480
52	$H_3Si-SiH_3$	-582.5741289	-582.5775540	-582.6461184	-582.5689140
53	CH_3Cl	-500.1110837	-500.1407176	-500.1587838	-500.1240486

54	H_3C-SH	-438.6993453	-438.7227833	-438.7522481	-438.7115054
55	HOCl	-535.9991192	-536.0077605	-536.0210971	-535.9776789
56	SO_2	-548.7029879	-548.6889018	-548.7123989	-548.6459441
57	BF_3	-324.6584412	-324.5968127	-324.6901858	-324.5784263
58	BCl_3	-1405.6067787	-1405.6781319	-1405.6716959	-1405.6106713
59	AlF_3	-542.3013387	-542.2265324	-542.3326319	-542.1962662
60	$AlCl_3$	-1623.2934005	-1623.3501754	-1623.3634275	-1623.2744029
61	CF_4	-437.6219573	-437.5522985	-437.6560419	-437.5211598
62	CCl_4	-1878.9322464	-1879.0191838	-1879.0072055	-1878.9245199
63	O=C=S	-511.5925738	-511.5939239	-511.6145182	-511.5590992
64	CS_2	-834.5374208	-834.5633474	-834.5680882	-834.5146597
65	COF_2	-313.1151396	-313.0683760	-313.1373305	-313.0416603
66	SiF_4	-689.2803701	-689.1894468	-689.3222617	-689.1524769
67	$SiCl_4$	-2130.5597966	-2130.6465755	-2130.6486830	-2130.5457982
68	N_2O	-184.7244871	-184.7069177	-184.7269723	-184.6789031
69	ClNO	-590.1595795	-590.1618536	-590.1674082	-590.1149080
70	NF_3	-354.2129288	-354.1530031	-354.2192528	-354.1156233
71	PF_3	-641.1076999	-641.0465333	-641.1354196	-641.0074450
72	O_3	-225.5127700	-225.4743282	-225.4934082	-225.4333402
73	F_2O	-274.7685338	-274.7124703	-274.7623493	-274.6790295
74	ClF_3	-759.6499228	-759.6072973	-759.6568800	-759.5488444
75	C_2F_4	-475.6581809	-475.5843171	-475.6968752	-475.5481140
76	C_2Cl_4	-1917.0285107	-1917.1164254	-1917.1136117	-1917.0190584
77	CF_3CN	-430.5730074	-430.5114790	-430.6135497	-430.4772993
78	C_3H_4 (propyne)	-116.6420882	-116.6482855	-116.6999367	-116.6524173
79	C_3H_4 (allene)	-116.6469682	-116.6530942	-116.7034171	-116.6563376
80	C_3H_4 (cyclopropene)	-116.6029698	-116.6179632	-116.6624054	-116.6216086
81	C_3H_6 (propylene)	-117.8788902	-117.8917469	-117.9534183	-117.9030059
82	C_3H_6 (cyclopropane)	-117.8613115	-117.8825966	-117.9390554	-117.8944388
83	C_3H_8 (propane)	-119.0966510	-119.1169584	-119.1882367	-119.1355443
84	C_4H_6 (butadiene)	-155.9676270	-155.9779427	-156.0515670	-155.9864850
85	C_4H_6 (2-butyne)	-155.9520195	-155.9644249	-156.0366480	-155.9731815
86	C_4H_6 (methylene cyclopropane)	-155.9327196	-155.9524940	-156.0192634	-155.9610947
87	C_4H_6 (bicyclobutane)	-155.9122183	-155.9410587	-156.0020899	-155.9501875
88	C_4H_6 (cyclobutene)	-155.9393749	-155.9603949	-156.0273546	-155.9696091
89	C_4H_8 (cyclobutane)	-157.1608590	-157.1878499	-157.2663245	-157.2048790
90	C_4H_8 (isobutene)	-157.1837015	-157.2015017	-157.2853948	-157.2178002
91	C_4H_{10} (trans butane)	-158.3961527	-158.4214867	-158.5148851	-158.4450886
92	C_4H_{10} (isobutane)	-158.3968774	-158.4216410	-158.5158591	-158.4454812
93	C_5H_8 (spiropentane)	-195.2216439	-195.2550240	-195.3388126	-195.2693197
94	C_6H_6 (benzene)	-232.2159155	-232.2293224	-232.3272213	-232.2362790
95	H_2CF_2	-239.0461450	-239.0135505	-239.0803682	-239.0018863
96	HCF_3	-338.3369176	-338.2854298	-338.3706058	-338.2637493
97	H_2CCl_2	-959.7230439	-959.7724428	-959.7800931	-959.7298505
98	$HCCl_3$	-1419.3312248	-1419.3997341	-1419.3972541	-1419.3310777
99	H_3C-NH_2 (methylamine)	-95.8465492	-95.8540531	-95.8999190	-95.8615570
100	CH_3-CN (methyl cyanide)	-132.7561971	-132.7559175	-132.8026262	-132.7534316
101	CH_3-NO_2 (nitromethane)	-245.0706549	-245.0508927	-245.1067642	-245.0303036
102	CH_3-O-N=O (methyl nitrite)	-245.0660761	-245.0421635	-245.1012242	-245.0215117
103	CH_3-SiH_3 (methyl silane)	-331.1924909	-331.2002524	-331.2610473	-331.2032076
104	HCOOH (formic acid)	-189.8096228	-189.7896725	-189.8401095	-189.7769669
105	$HCOOCH_3$ (methyl formate)	-229.0976810	-229.0798631	-229.1545052	-229.0721663
106	CH_3CONH_2 (acetamide)	-209.2326569	-209.2275613	-209.3014959	-209.2256427
107	CH_2-NH-CH_2 (aziridine)	-133.9080037	-133.9219190	-133.9734105	-133.9268304
108	NCCN (cyanogen)	-185.6914447	-185.6745661	-185.7151356	-185.6534272
109	$(CH_3)_2NH$ (dimethylamine)	-135.1379480	-135.1498205	-135.2181407	-135.1621935
110	CH_3-CH_2-NH_2 (trans ethylamine)	-135.1492733	-135.1618458	-135.2296120	-135.1742418
111	H_2C=C=O (ketene)	-152.6272012	-152.6184945	-152.6616137	-152.6094434
112	CH_2-O-CH_2 (oxirane)	-153.7942676	-153.7967050	-153.8479205	-153.7956501
113	CH_3CHO (acetaldehyde)	-153.8395663	-153.8364222	-153.8916393	-153.8352512
114	O=CH-CH=O (glyoxal)	-227.8686394	-227.8463713	-227.9078597	-227.8304003
115	CH_3CH_2OH (ethanol)	-155.0348458	-155.0364177	-155.1047564	-155.0436248

116	CH_3-O-CH_3 (dimethylether)	-155.0192811	-155.0189886	-155.0883805	-155.0260157
117	CH_2-S-CH_2 (thiooxirane)	-476.7804087	-476.8098115	-476.8454283	-476.7960552
118	CH_3CH_3SO (dimethyl sulfoxide)	-553.2234450	-553.2391660	-553.3040129	-553.2232633
119	CH_3-CH_2-SH (ethanethiol)	-477.9996024	-478.0280824	-478.0795751	-478.0217614
120	CH_3-S-CH_3 (dimethyl sulphide)	-477.9994813	-478.0281654	-478.0787183	-478.0213625
121	H_2C=CHF	-177.8507010	-177.8370945	-177.8958862	-177.8328630
122	CH_3-CH_2-Cl (ethyl chloride)	-539.4145939	-539.4491682	-539.4893191	-539.4374422
123	H_2C=CHCl (vinyl chloride)	-538.1932844	-538.2213453	-538.2504971	-538.2018126
124	H_2C=CHCN (acrylonitrile)	-170.8368251	-170.8339218	-170.8921784	-170.8284787
125	CH_3-CO-CH_3 (acetone)	-193.1508099	-193.1526423	-193.2302345	-193.1566161
126	CH_3COOH (acetic acid)	-229.1213555	-229.1065645	-229.1795506	-229.0991850
127	CH_3COF (acetyl fluoride)	-253.1453253	-253.1221847	-253.1955780	-253.1105157
128	CH_3COCl (acetyl chloride)	-613.4791286	-613.4959933	-613.5393020	-613.4682453
129	$CH_3CH_2CH_2Cl$ (propyl chloride)	-578.7141615	-578.7537841	-578.8160480	-578.7470777
130	$(CH_3)_2CH$-OH (isopropanol)	-194.3392226	-194.3453202	-194.4364060	-194.3576881
131	C_2H_5-O-CH_3 (methyl ethyl ether)	-194.3239742	-194.3286942	-194.4201876	-194.3407155
132	$(CH_3)_3N$ (trimethylamine)	-174.4317314	-174.4470053	-174.5388781	-174.4645291
133	C_4H_4O (furan)	-230.0281248	-230.0275046	-230.1050253	-230.0235037
134	C_4H_4S (thiophene)	-553.0062397	-553.0336067	-553.0934141	-553.0159508
135	C_4H_4NH (pyrrole)	-210.1566013	-210.1673769	-210.2454971	-210.1694771
136	C_5H_5N (pyridine)	-248.2690786	-248.2753195	-248.3682226	-248.2753987
137	SH	-398.7564278	-398.7705862	-398.7771159	-398.7527721
138	CCH	-76.6094809	-76.6093721	-76.6349396	-76.6064028
139	C_2H_3 (^{2}A')	-77.8934833	-77.8983780	-77.9339874	-77.9018427
140	CH_3CO (^{2}A')	-153.1977123	-153.1916992	-153.2411975	-153.1866245
141	H_2COH (^{2}A)	-115.0751211	-115.0686004	-115.1101260	-115.0675088
142	CH_3O (^{2}A')	-115.0631056	-115.0559114	-115.0988710	-115.0551174
143	CH_3CH_2O (^{2}A")	-154.3625947	-154.3604736	-154.4254657	-154.3646301
144	CH_3S (^{2}A')	-438.0615424	-438.0810089	-438.1075559	-438.0670729
145	C_2H_5 (^{2}A')	-79.1325273	-79.1443811	-79.1898785	-79.1551219
146	$(CH_3)_2CH$ (^{2}A')	-118.4386967	-118.4560703	-118.5225751	-118.4713658
147	$(CH_3)_3C$	-157.7442423	-157.7667611	-157.8549570	-157.7868459
148	NO_2	-205.1534326	-205.1283536	-205.1521206	-205.0974391